

Popular summary: "A Comparison of the Stratospheric Age-Spectra from Data Assimilation Models and Implications for the Transport of Trace Gases"

This paper analyzes the transport properties of the meteorological data sets that are now widely used for the transport of trace gases in 3D models of stratospheric ozone models. These 3D models are being used for ozone layer assessment purposes, and in climate models for the stratospheric transport of aerosols.

We have found a number of serious problems with the meteorological data sets. The most serious is that the tropical stratosphere is not very isolated from mid-latitudes (contrary to observations). This means that CFC's and other gases, which enter the stratosphere in the tropics, would move too quickly to mid-latitudes and probably exit the stratosphere before releasing the chlorine. Observations of long lived trace gases show that this doesn't happen.

The analyses show that the excessive tropical ventilation of the stratosphere appears to be endemic to assimilation meteorological analyses. We show also that the general circulation model (GCM) upon which the assimilation is based does not exhibit the tropical ventilation problem. We speculate that improved tropical physics in the GCM would reduce the tropical ventilation.

A Comparison of the Age-Spectra from Data Assimilation Models

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Abstract

We use kinematic and diabatic back trajectory calculations, driven by winds from a general circulation model (GCM) and two different data assimilation systems (DAS), to compute the age spectrum at three latitudes in the lower stratosphere. The age-spectra are compared to chemical transport model (CTM) calculations, and the mean ages from all of these studies are compared to observations. The age spectra computed using the GCM winds show a reasonably well-isolated tropics in good agreement with observations; however, the age spectra determined from the DAS differ from the GCM spectra. For the diabatic trajectory calculations, the age spectrum is too broad as a result of too much exchange between the tropics and mid-latitudes. The age spectrum determined using the kinematic trajectory calculation is less broad and lacks an age offset; both of these features are due to excessive vertical dispersion of parcels. The tropical and mid-latitude mean age difference between the diabatically and kinematically determined age-spectra is about one year, the former being older. The CTM calculation of the age spectrum using the DAS winds shows the same dispersive characteristics of the kinematic trajectory calculation. These results suggest that the current DAS products will not give realistic trace gas distributions for long integrations; they also help explain why the mean ages determined in a number of previous DAS driven CTM's are too young compared with observations. Finally, we note trajectory-generated age spectra show significant age anomalies correlated with the seasonal cycles, and these anomalies can be linked to year-to-year variations in the tropical heating rate. These anomalies are suppressed in the CTM spectra suggesting that the CTM transport is too diffusive.

1. Introduction

One of the goals of data assimilation is to produce a meteorological analysis realistic enough to enable chemical modelers, using chemical transport models (CTM's) and observations, to diagnose the chemical reaction system [Rood et al., 1989]. While it is generally agreed that steady improvement in assimilation systems has been made, the simulation of long lived tracer fields by assimilation systems continues to show

significant biases [Douglass et al., 2001, 2002]. The goal of this paper is to examine the overall stratospheric transport properties of two data assimilation systems (DAS), and the underlying core general circulation model (GCM) of one of them, with the intent of explaining the differences between the simulations and observations. The approach we take is to compute the age spectrum at selected points within the stratosphere and from the spectrum compute the mean age for comparison with observations.

The age of air concept is reviewed in Waugh and Hall [2002]. The age-spectrum is the probability distribution function of the transit times of parcels from a source region to the sample region. The age-spectrum, thus defined, is a function of both time and space, and contains all the information on the transit times between the entry of air into the stratosphere and its appearance at a given coordinate. The age spectrum can be connected to the chemical distribution of both long and short-lived gases [Hall and Plumb, 1994; Holzer and Hall, 2000, Schoeberl et al., 2000]. The mean age is the first moment of the age spectrum.

Hall and Plumb [1994] showed that for a stationary circulation, the age spectrum may be determined by plotting the evolution of a long lived trace gas in a pulse release experiment. Likewise for a stationary circulation with a linearly increasing source gas (e.g. CO₂, SF₆), the mixing ratio can be directly related to the mean age. Thus the chemical model computed mean age can be compared to observations [Waugh et al. 1997; Holzer and Hall, 2000].

The stationarity assumption means that the age spectrum is only a function of the transit time. That is, the age-spectrum is assumed to be independent of the actual point in time that the spectrum is computed. To first order, the stratospheric circulation can be considered nearly stationary: air rises in the tropics and descends at mid-latitudes. Indeed the characterizations of stratospheric transport as a simple diffuser [Plumb and Ko, 1992] or a “tropical pipe” [Plumb, 1996; Shia et al., 1998] or “leaky tropical pipe” [Neu and Plumb, 1999] imply that to first order the transport system can be approximated by a simple, stationary circulation. However, our calculations show that the departure from stationarity becomes larger away from the lower tropical stratosphere due to seasonal and interseasonal variations. Thus the pulse gas release method of computing the age spectrum becomes increasingly inaccurate away from the source region for a non-stationary flow [Holzer and Hall, 2000]. A more appropriate choice for age spectrum computation is the trajectory calculation. In the trajectory method, a large number of parcels are released and integrated backward or forward in time until they interact with the source region (typically the tropopause). The trajectory method allows the computation of the exact age spectrum, $G(x,y,z,\tau,t)$, where τ is the transit time and the other variables have their usual meaning. The trajectory method does not rely on the flow being stationary.

The forward trajectory approach, as used by Eluszkiewicz et al. [2000] (hereafter E2000), parcels are continuously released at the tropical tropopause and then removed when they re-enter the troposphere. Once the system has reached steady state, the histogram of parcel “ages” for a given location is the age spectrum. The disadvantage of the forward

trajectory technique is that in trajectory models, the parcel density decreases with altitude at roughly the same rate as the atmospheric density. Thus the calculation requires a very large number of parcels to be forward integrated for a long time so that the age spectrum can be resolved high altitudes.

With backward trajectory calculations, parcels are initialized in a small volume and the model is run backward in time until the parcels have crossed into the troposphere. The spectrum is computed from the transit times. Unlike the forward trajectory approach, the results from backward trajectory calculations are statistically robust, but are still computationally expensive since the whole calculation has to be repeated for every grid point and time. In this paper we will use the backward trajectory approach but limit ourselves to three latitudes. It should be noted, however, that if the circulation is not stationary, the forward and backward trajectory approaches yield different results.

This paper follows two important works that have also looked at the mean ages computed for models. In the first, Hall et al. [1999] computed the mean age for a large number of 2-D and 3-D models to assess their transport characteristics. The model mean ages were computed from the age spectrum as derived from pulse gas experiments for each model. Hall et al. [1999] classified the models based upon the age distribution as having too much (Class A) or too little (Class C) tropical isolation. Among the models tested, nearly all showed too young a mean age suggesting excessive vertical transport or excessive mixing of mid-latitude air into the tropics.

The second, E2000, focused on the transport schemes themselves using GCM winds. E2000 compared the transport of a "Pinatubo" type tracer release with various Eulerian including second and fourth order schemes, upstream difference schemes, semi-Lagrangian schemes and trajectory calculations. E2000 found that the computed age of air was sensitive to the type of scheme used. They also noted that a diabatic trajectory calculation produced the most reasonable transport simulation. E2000 also found that if the trajectory model used the GCM vertical velocities instead of diabatic heating rates, the tracer transport showed significant vertical dispersion of parcels. Although the enhanced vertical dispersion associated with kinematic trajectory calculations has been noted in the past, it has always been presumed to be a result of improper temporal sampling of the vertical velocity fields (i.e., aliasing high frequency gravity waves and turbulent motions). E2000, showed that the enhanced vertical dispersion occurred even if the trajectory calculation was made at the same time resolution as the GCM. They concluded that the vertical velocities and their interpolation to the trajectory points were too noisy and thus generated the excessive vertical dispersion. The development of finite volume GCMs [Lin 1997] has improved the vertical motion representation so we will revisit E2000's conclusion in this paper.

Below we will use the age spectrum generated using the trajectory method mainly as a diagnostic of the transport for a number of different assimilated meteorological and GCM data sets. The age spectrum can be used to compute the mean age, and these mean ages can be compared to observations as discussed in Hall et al. [1999]. As mentioned above, Hall et al. [1999] reported that models tend to underestimate the atmospheric age in the

lower stratosphere (15-30 km) at all latitudes compared to CO₂ and SF₆ estimates of the mean ages. However, the mean age only gives one piece of information about the age spectrum, and for a very skewed or multi-modal spectrum, the mean age poorly represents the transport information available in the age spectrum. As a case in point, examination of the spectrum produced in this study shows that some of the meteorological data sets produce reasonable mean ages despite obviously incorrect age spectra. In general, we will show that assimilated meteorological variables do not do a good job characterizing the lower stratospheric transport due to excessive ventilation of the tropics. On the other hand, the GCM we tested showed excellent transport characteristics. These results have broad important implications for assessments of the impact of natural and anthropogenic changes in trace gas concentrations on stratospheric composition and chemistry.

2. The Trajectory Generated Age-Spectrum

There are two types of trajectory models: diabatic and kinematic. The diabatic model describes parcels that are transported along isentropic surfaces by the large-scale wind field and moved across isentropic surfaces by the net diabatic heating. (The diabatic model becomes adiabatic or isentropic if the heating rate is set to zero.). In a kinematic trajectory model the horizontal transport of parcels takes place on pressure surfaces and the vertical motion across these surfaces is generated by the omega field (dp/dt). Ideally, the results of kinematic and diabatic models would be the same, but Danielson et al. [1961], using gridded analyses, first noted that noise in the omega field ($\omega=dp/dt$, where p is pressure), computed from the mass continuity equation, leads to very large errors in trajectory positions. Danielson obtained much more realistic results by constraining the parcels to move adiabatically. (Note also that even if the analyses fields were perfect, small differences in the formulation, combined with numerical inaccuracies, would lead to some small differences between the diabatic and kinematic methods.)

With the advent of regular gridded assimilated meteorological observations over the last fifteen years, trajectory models have increasingly been used to provide an assessment of the transport characteristics of the atmosphere especially the stratosphere. The accuracy of short-term trajectory calculations has been tested using observations, and for time scales of less than a week, trace gas anomalies computed using individual trajectories can be linked directly to observations (e.g. Waugh et al. [1994]). For longer time scales, the accuracy of an individual trajectory becomes questionable mainly due to the accumulated uncertainty in the meteorological fields [Schoeberl and Sparling, 1995]. This means that only the statistical properties of the trace gas fields calculated from longer trajectory integrations can be related to observations [Schoeberl et al., 2002, Rosenfield and Schoeberl, 2002, Manney et al., 1994].

If the trace gas distributions determined from long trajectory integrations are to provide a realistic statistical description of those in the real atmosphere, the analyzed meteorological fields must provide an unbiased representation of the flow. For example, if the divergent component of the analyzed dataset were excessive, the modeled trace gas distributions would not maintain the correct correlations with the potential vorticity field

over long periods. While there is evidence that most assimilated analyses are accurate enough for short-term integrations, the accumulation of small errors in these analyses result in significant biases in trace gas distributions over longer periods, as seen in chemical-transport model (CTM) studies of long-lived species [e.g. Douglass et al. 2002]. Biases in the analyzed circulation fields can exacerbate those biases that arise from inaccurate transport schemes in CTM's [E2000]. A central objective of this paper is to diagnose the process by which these biases are manifested.

The approach taken is to compare the age spectrum for several meteorological data sets at selected points. The age spectrum is computed by releasing 39,600 parcels along a zonal band (to relate to the zonal mean ages published in, for example, Hall et al. [1999]) 1° latitude wide and 10 K in potential temperature depth. Three release locations are used: 0 N, 460K; 40 N 440K; 70 N 440K (see Table 1). The trajectory model is integrated backward for 3000 days starting Jan 1, 2001. The parcel ensemble is evaluated every 10 days, and parcels 1/2 km below the local tropopause are removed. This procedure is the same as that used to evaluate long-term effluent aircraft effects in Schoeberl et al. [2000]. Those authors also examined the effect of terminating the parcel trajectories at lower altitudes. Lowering the removal height produced only a very small offset in the age spectrum demonstrating that parcels rapidly mixed downward once they enter the troposphere. Poleward of 15° the PV value of $2.0e-6$ K m²/kg/s is used to diagnose the tropopause. Equatorward of 15° , the tropopause is determined to be the lower of the height of the temperature minimum or the height of the 380 K isentrope. These heights are computed using spline interpolation of the temperature field onto a grid with 100m vertical spacing.

The age spectrum, G , is computed by generating a histogram of parcel ages. The histogram is then integrated and normalized so that the $\int G(t)dt = 1$. There is some ambiguity in the estimate of $G(t)$ because for many experiments not all the parcels have left the stratosphere after 3000 days of integration. We overcome this problem by fitting the distribution to an exponential decay rate for the last four years to extend the spectrum until no parcels remain in the stratosphere. This procedure is suggested by the long-time approximation of the Green's function for the diffusion problem [Hall and Plumb, 1994, Eq. 21]

2.1 The GCM model and the DAS

For these experiments, two DAS models were tested: the United Kingdom Meteorological Office (UKMO) model [Swinbank and O'Neill, 1994], and the Finite-Volume Data Assimilation System (FVDAS) model. The UKMO assimilation system has provided a continuous set of data following the launch of the Upper Atmosphere Research Satellite in September 1991. The UKMO DAS has a horizontal resolution of $3.75^\circ \times 2.5^\circ$ (lon., lat.), extends to 0.4 hPa, and the data are reported once a day. The heating rates are not reported for UKMO so we compute these off-line as described in Rosenfield et al. [1994]. These heating rates include only long and short wave fluxes.

The Finite Volume General Circulation Model (FVGCM) was developed in collaboration with the National Center for Atmospheric Research (NCAR). The FVGCM model uses a flux-form semi-Lagrangian transport scheme [Lin and Rood, 1996, 1997] and a quasi-Lagrangian vertical coordinate system [Lin, 1997], which ensures accurate representation of transport by the resolved-scale flow. The FVGCM has a horizontal resolution of $2.5^\circ \times 2^\circ$ (lon., lat.), extends to 0.01 hPa, and the daily averaged product is available to the user. Physical parameterizations in the current version of the FVGCM are from the NCAR Community Climate Model, Version 3 (CCM3), described by Kiehl et al. [1998]. A 35 year run of the FVGCM has been performed by NASA's Data Assimilation Office (DAO). Note that the FVGCM fields correspond to no particular year unlike the DAS fields. Our back integrations were performed by taking the year 2001 to be year 11 of the FVGCM run.

The Finite Volume Data Assimilation System (FVDAS) is a new observational assimilation system produced by the DAO. The core of FVDAS uses the FVGCM. The FVDAS has the same horizontal resolution as the FVGCM but extends only to 0.4 hPa, and the FVDAS fields are available every six hours. The FVDAS assimilation system uses the Physical-Space Statistical Analysis Scheme (PSAS) [Cohn et al., 1998]. Since there were only two years of FVDAS data, 1999 and 2000, at the time of this study, we have created an artificial periodic "year 1999" data set which is one year and one month in length, by smoothly nudging the data at the beginning of 1999 so that it merges with then beginning of year 2000. This periodic form of the FVDAS data was used for the long integrations needed to produce the age spectrum. The diabatic heating rates for the FVDAS include latent heat release as well as the heating due to short wave and long wave flux convergence of radiation.

The kinematic trajectory model uses the same base trajectory code as the diabatic model [Schoeberl et al., 2000] except that the omega field is used to move the particles vertically, instead of the diabatic heating. Both the UKMO and DAO provide omega as a diagnostic from their assimilation systems, but there are some differences in both the methods used to calculate omega in the two systems and in the averaging applied. The UKMO system is like most present GCM models, in that the vertical velocities are determined numerically, using the horizontal mass divergence and an "omega-equation" approach. In order to suppress the noise, temporal smoothing is applied before omega is used in the trajectory calculation. In the FVDAS (and FVGCM), omega is calculated in a different manner. Lin (1997) describes the use of a quasi-Lagrangian vertical coordinate, where the fluid equations are solved on material surfaces, from which a direct computation of vertical velocity is made: it is simply the rate of change of mean pressure of the grid box. This approach leads to a much smoother omega field that is less prone to numerical round-off errors than traditional approaches.

To link our results to chemical transport experiments, we have computed the age spectrum using the 3D chemical transport model (CTM) [Douglass et al., 2001] using the winds and temperatures from UKMO DAS. The CTM does not use the time smoothed omega fields from the assimilation, but computes omega from the divergence equation using the assimilated u and v fields to insure mass conservation. To compute the age

spectrum, we placed a passive tracer source at 200 hPa from 5°S to 5°N. The thickness of the source region is about 60 hPa. After the first month of integration, the source is turned off, and a tracer sink from 5°S to 5°N is created at the ground by specifying the mixing ratio to be zero. The CTM is run from Jan 1, 1992 to July 1, 1997. This a shorter period than the trajectory runs, but it is long enough to produce an accurate age spectrum as will be shown below. We have also used the CTM to compute the mean ages for the FVGCM and FVDAS, with an SF₆ – type experiment [Hall et al., 1999]. In this experiment we use a time increasing passive tracer source like SF₆ to compute the mean age directly. Table 1 summarizes all the experiments.

General comparison of the trajectory and CTM results with observations can be made using the mean age computed using SF₆ and CO₂ observations. Here we use the lower stratospheric mean age reported by Hall et al. [1999] as indicated in the Obs. category in Table 1 and shown in Fig. 9.

Table 1. Summary of the experiments performed for this study. The columns of the table denote the experiment name, followed by the characteristics (kinematic or diabatic trajectories, or other techniques; the latitude and potential temperature of the reference point; the meteorological datasets used) and showing the mean age calculated in the experiment.

Exp.	Type	Lat. (deg N)	Initial PT	Met. Fields	Mean age (yr)
460_0du	Diabatic	0	460K	UKMO	2.2
460_0ku	Kinematic	0	460K	UKMO	0.74
460_0da	Diabatic	0	460K	FVDAS	2.3
460_0ka	Kinematic	0	460K	FVDAS	0.86
460_0kg	Kinematic	0	460K	FVGCM	0.92
CTM	Pulse Exp,	0	460K	UKMO	1
CTM	SF ₆	0	460K	FVDAS	0.43
CTM	SF ₆	0	460K	FVGCM	0.84
Obs.		0	~460K		1.1
460_40du	Diabatic	40	440K	UKMO	2.7
460_40ku	Kinematic	40	440K	UKMO	1.8
460_40da	Diabatic	40	440K	FVDAS	2.9
460_40ka	Kinematic	40	440K	FVDAS	1.6
460_40kg	Kinematic	40	440K	FVGCM	1.9
CTM	Pulse	40	440K	UKMO	1.36
CTM	SF ₆	40	440K	FVDAS	1.47
CTM	SF ₆	40	440K	FVGCM	2.42
Obs		40	~440K		3.5-4.
440_70du	Diabatic	70	440K	UKMO	3.6
440_70ku	Kinematic	70	440K	UKMO	2.3
440_70da	Diabatic	70	440K	FVDAS.	3.8
460_70ka	Kinematic	70	440K	FVDAS	2.6
440_70kg	Kinematic	70	440K	FVGCM	3.5
CTM	Pulse	70	440K	UKMO	1.52
CTM	SF ₆	70	440K	FVDAS	1.95
CTM	SF ₆	70	440K	FVGCM	3.72
Obs.		70	~440K		4-4.5

3. Results

3.1 Tropics

Figure 1 shows a snap shot of the five equatorial trajectory simulations (Table 1, Exps. 460_0..) after 50 and 200 days of backward integration. (Note that since these are backward integrations, Fig. 1b shows descending relative to the Fig. 1a. In a forward integration the parcels would be rising in response to tropical heating.)

The two diabatic simulations, using assimilated winds from UKMO and the FVDAS, show parcels rapidly moving to middle latitudes after 50 days. The diabatic distributions are generally similar even after 200 days although the FVDAS integration is beginning to show an upward plume in the north polar region not seen in the UKMO case. In contrast, the UKMO and FVDAS kinematic integrations show large vertical dispersion of parcels after 50 days; some parcels have already moved into the troposphere and have been removed from the model. Strikingly, the FVGCM kinematic integration shows almost no meridional or vertical dispersion after 50 days and the distribution is still confined to middle and low latitudes after 200 days, while the four DAS experiments have moved parcels to the polar regions.

Figure 2 shows the age spectrum for these simulations as well as the CTM results. In combination with Fig. 1, interpretation of these spectra is straightforward. First, there is almost no offset from zero age for the UKMO and FVDAS kinematic calculations. The lack of offset is due to the strong vertical dispersion shown in Fig. 1 that puts parcels into the troposphere almost immediately. The net result of this dispersion is to bias the mean age toward the young side. Remarkably the other simulations all show nearly the an offset value of about six months. The strong zonal mean dispersion of parcels is equivalent to diffusion in a 2D sense since it implies rapid vertical mixing of fluid elements. From the vertical dispersion of the parcels shown in Fig. 1 we estimate an equivalent 2D vertical diffusion rate of $\sim 1\text{m}^2/\text{sec}$. This rapid vertical dispersal of parcels is 50 times larger than the observational constraints imposed by, for example, water vapor observations [Mote et al., 1998] and is thus unrealistic.

The modal peaks of the tropical spectra calculated from the diabatic trajectory calculations are in good agreement with each other and with the FVGCM calculation. The strong vertical dispersion of the kinematic trajectory parcels is not present in the diabatic calculations. This difference between diabatic and kinematic trajectories is consistent with the results obtained by Mahowold et al. [2002]. They showed that a hybrid isentropic-sigma coordinate system (isentropic in the stratosphere) produced reduced vertical diffusion compared to the sigma-only model.

Away from the peaks, the age spectra generated by the diabatic trajectories using the DAS winds show long tails compared to the FVGCM. The explanation for this is also seen in Fig. 1. The diabatic assimilations show virtually no tropical barrier to transport and thus rapidly mix mid-latitude air and tropical air. This mixing process brings in older

mid-latitude air into the tropical parcel distribution producing a long tail on the age spectrum. Ventilation of the tropics also increases the age of the whole system because parcels can circulate between the tropics and mid-latitudes, ascending and descending, increasing their stratospheric lifetime. This effect was also noted in the “leaky tropical pipe” model of Neu and Plumb [1999]. In contrast with the DAS simulations, tropical air in the FVGCM is equatorially confined, so the tail of the FVGCM age spectra falls off more rapidly.

Within the long tails of the diabatic DAS age spectra, there are peaks roughly lined up with the late winter periods in the northern and southern hemispheres. For the FVDAS case the peaks are regular and decreasing in amplitude because we are recycling one year of data. This is not true of the UKMO simulations; particularly dramatic is the peak at three years in the UKMO diabatic experiment. This peak is ~20% the size of the modal peak. Figure 3 shows the time series of the lower stratosphere, equatorial, diabatic heating rate used by the UKMO diabatic trajectory code. Note the higher diabatic heating values for the winter of 1998 corresponding to colder tropopause temperatures. The enhanced diabatic heating would correspond to increased injection of air and increase the amount of lower stratospheric air with that age, as is seen in the spectrum. To check whether this 1997/8 heating is responsible for the peak, we ran a second trajectory integration starting on Jan 1, 2000 (one year earlier). The results of this integration are not shown, but the secondary large peak for that integration appears one year earlier as would be expected if the peak were due to the higher heating rate in 1997/8.

The CTM tracer pulse generated age spectrum is shown in Fig. 2. This spectrum also shows a lack of offset and an early modal peak as expected since the CTM vertical motion is computed from the divergence of UKMO wind fields and is more or less equivalent to the kinematic trajectory calculation. The CTM age spectrum decays more slowly than the kinematic trajectory computation. We hypothesize that the slower decay of the CTM spectrum is a result of transport-algorithm diffusion across grid cells (see E2000). The transport scheme will diffuse tracer between grid cells thus sharp gradients in the age will be reduced and this will have the effect of erasing the structure of the age spectrum.

Mean age comparisons with observations will be discussed below with the presentation of Fig. 9, but it is appropriate to comment here on the discrepancy between the mean ages shown in Fig. 2. The mean ages of the FVGCM, the CTM and the kinematic trajectory spectra all are in reasonable agreement; however, the diabatic mean ages are nearly a year older than the other simulations. The diabatic trajectory mean ages are old because of the long spectral tails produced by the lack of a tropical barrier, and the presence of an age offset in the front of the spectrum. The FVGCM age is younger than the diabatic ages, even though it also has an age offset, simply because the spectral tail is shorter. In the case of the kinematic trajectories and the CTM, the vertical dispersion of the parcels both shorten the spectral tail and remove the offset. The kinematic trajectory calculations also display a lack of a tropical barrier, but it is the enhanced vertical dispersion that mitigates that result of tropical ventilation. In other words, even though the DAS meteorological

fields lack a tropical transport barrier, the kinematic trajectory and CTM calculations have so much vertical dispersion that the tropical transport effect is masked, and the result is a reasonable mean age. Using diabatic heating rates rather than the omega field clearly suppresses the excessive vertical dispersion, but it does not solve the problem of excessive ventilation of the tropics.

The lack of a tropical transport barrier in the DAS is unrealistic. Tropical trace gas observations show that the region is weakly isolated from mid-latitudes just above the tropopause with an increasing amount of isolation with altitude into the mid-stratosphere [Avallone and Prather, 1996, Minshwaner et al., 1996; Volk, et al., 1996; Mote et al., 1998; Trepte and Hitchman, 1993; Grant et al., 1996; Schoeberl et al., 1997]. The very existence of the quasi-biennial oscillation (QBO) requires isolation of the tropical region from mid-latitudes [Dunkerton, 1991, Baldwin et al., 2001]. Thus FVGCM represents the isolation of the tropical stratosphere most realistically.

3.2 Mid-latitudes

Figure 4 shows the snap shots of the mid-latitude release (Table 1, Exps. 440_40..) at 50 and 200 days back integration. At 50 days the UKMO and FVDAS kinematic experiment again show large vertical parcel dispersion. The two diabatic experiments show less vertical dispersion but do show parcels extending along potential temperature surfaces into the tropics. The DAS experiments all show more dispersion than the FVGCM experiment. At 200 days all the DAS experiments show parcels extending into the high southern latitudes where the FVGCM parcels are confined mostly to the northern latitudes and the tropics.

After 200 days, two diabatic DAS experiments differ at high northern latitudes. The FVDAS (third panel) shows more parcels moved to higher altitudes than UKMO (first panel). Figure 5 shows a plot of the 70°N heating rates and assimilated temperatures for the UKMO and FVDAS. Note that the UKMO heating rates are diagnosed from the temperature field while the FVDAS is a model output product. Fig. 5 shows that the high altitude summer heating (above 35 km) in the UKMO DAS has a higher magnitude and extends over a longer time period than the FVDAS, and the FVDAS net heating fields show cooling almost throughout the entire summer period. This means that there will be more descent for the FVDAS parcels. From a back trajectory viewpoint, this means FVDAS parcels will be lofted higher than UKMO parcels which explains the plume of upward moving parcels in Fig. 4b (third panel). We note that the UKMO temperature fields are slightly cooler than the FVDAS. The cooler temperatures would reduce the net cooling rate since the cooler temperatures are closer to radiative equilibrium. It should be noted that these kinds of polar transport differences between the two DAS fields will produce quite different estimates in the chemical composition in the polar vortex [Rosenfield and Schoeberl, 2001].

Figure 6 shows the age spectrum for the mid-latitude release experiments. Compared to Fig. 2, the spectra are very broad, as might be expected since parcels released in mid-latitudes will have to enter the tropics to be removed (in the back-trajectory sense).

Because of the longer travel paths, there is increased opportunity for parcels to be circulated in and out of the tropics which will have the effect of broadening the spectrum even further. As with the tropical case, there is almost no offset for the UKMO and FVDAS kinematic experiments. Again this is clearly the result of the strong vertical dispersion of parcels (Fig. 6a) which unrealistically enter the troposphere at mid-latitudes giving low age values. Fig. 6 (also Table 1) shows that the two diabatic experiments are quite close in their estimates of the mean age, but both are nearly a year older than the other experiments. Again, we see the compensating effects in the DAS experiments of vertical dispersion, which tends to make the mean age younger due to lack of an age offset. To repeat the important conclusion from the previous section: Both biases from both vertical and horizontal dispersion are playing a role in the kinematic experiments, but in the diabatic experiments only biases from horizontal dispersion are significant. The FVGCM shows reduced levels of both horizontal and vertical dispersion.

Finally we note that the CTM result produces the youngest mean age and the smoothly decaying age spectrum with no significant secondary peaks. In contrast, the year three peak in the UKMO diabatic spectrum is now nearly as large as the modal peak. This suggests at least two pathways for parcels to reach the 40° latitude, a straight path from the tropics, and a higher altitude path. Multiple paths are suggested by the results of observational results of Andrews et al. [2001] and the modeling study of Schoeberl et al. [2000].

3.3 Polar

Figure 7 shows the snap shots of the polar release after 200 days. Because of the stronger temperature variation with longitude, the 440 K release takes place over a wider altitude range than the mid-latitude and tropical experiments. In most other respects the parcel dispersion is similar to the mid-latitude experiment except the DAS experiments show a little less cross tropical penetration after 200 days. The two diabatic assimilations differ, as before, in the appearance of a strong upward plume in the polar region for the FVDAS compared to UKMO. This feature was discussed the last section.

Figure 8 shows the age spectrum for the polar experiment. The UKMO and FVDAS kinematic spectra again show the lack of offset. Even though the release is at high latitudes the vertical dispersion quickly propels some parcels across the tropopause. All of the trajectory age spectra (except the CTM) show the lack of a clear modal peak characteristic of the previous experiments, and the spectral decay rates are so slow that it may not be possible to define a mean age. ($G(\tau)$ must decay faster than $1/\tau$ for the mean age integral to converge.) The lack of a large modal peak is consistent with the findings of Rosenfield and Schoeberl [2001] that polar air consists of both air that has descended from high altitudes and air that has been entrained by the formation of the vortex. This simply means that there are many paths air parcels can take into the vortex. Note that the three-year age peak, seen in the FVDAS mid-latitude and tropical simulations, has now become the modal peak.

3.5 Comparison of mean ages

Figure 9 shows the CTM computed mean age for the FVDAS and the FVGCM, the trajectory computed mean ages for the experiments shown in Table 1 along with ages computed from ER-2 observations of CO₂ [Boering et al., 1996] and SF₆ [Elkins et al. 1996] from Hall et al. [1999]. The observed ages referenced to the mean tropical tropopause and are thus consistent with the computed ages shown here.

As noted above, the tropical DAS and FVGCM kinematic trajectory mean ages agree fairly well with each other and with the observations; however, the DAS diabatic trajectory ages are too old. There is also good agreement between the FVGCM kinematic trajectory mean age and the FVGCM CTM mean age. Interestingly, the FVDAS CTM mean age is fairly young, and is not in agreement with the FVDAS kinematic mean age – although they are close. The explanation for this difference is not evident. We note also that the UKMO CTM pulse experiment actually gives an older age than the kinematic trajectory experiment (Table 1). One possible explanation is that the steady increasing source gas method of determining the mean age is not equivalent to the pulse method due to the gradient dependent numerics of the transport scheme. Grid cell diffusion would create slightly older ages in the pulse CTM experiment as older air diffuses into tropical cells toward the end of the integration period. On the other hand in the pulse experiment, the cell diffusion would always reduce the vertical gradient in the tropics increasing the SF₆ values in the cells which would be interpreted as younger air. It is clear that further study of the numerics of the transport schemes, as in E2000, is warranted.

Comparing mid-latitudes mean ages, all of the results show too young mean ages compared to observations; however, the diabatic calculations show better agreement than the kinematic calculations. From the results presented above, the young mid-latitude ages for the kinematic DAS calculations are a result of the rapid dispersion of parcels in the vertical. The relatively older ages for the diabatic DAS calculations are a result of the suppression of this vertical dispersion, but the diabatic ages are still too young because of excessive circulation of air into the mid-latitudes from the tropics. It is clear that an even older mean age could be achieved if the tropical barrier was not as permeable because parcels would have to ascend to enter the tropics at higher altitudes and then descend again to the tropopause which would increase their age. However, increasing the tropical barrier strength does not automatically increase the age gradient [Neu and Plumb, 1999], in addition, the strength of the stratospheric circulation would have to weaken to increase the mean age. Finally, we note that despite the reduced vertical dispersion of parcels in the FVGCM tropical experiments, vertical parcel dispersion appears to still play a role in reducing the mean age at mid-latitudes.

Moving to higher latitudes, we have good agreement between observations, the diabatic trajectories and the FVGCM results. This result suggests that the FVGCM and the diabatic trajectories calculations show fairly good agreement with observations. The isolation of the vortex in the FVGCM is well maintained. Figure 7 also shows that few FVGCM parcels directly enter the troposphere so the age spectrum is not contaminated by dispersal of parcels directly across the tropopause.

There is no corresponding CTM DAS experiment in this study which uses diabatic heating to move the trace gas vertically although such models have been developed [Chipperfield, 1999]. Our trajectory result predicts that diabatic transport using assimilated winds will produce much older tropical ages due to tropical – mid-latitude exchange.

3.6 Tropical PV flux

As a final check on our result that the DAS tropics are excessively ventilated, and to guarantee that this is not a result of some numerical problem the transport calculations, Figure 10 shows the January zonal mean modified potential vorticity flux $\overline{(v'q_m')}$ ($q_m' = q (\theta/\theta_0)^{-9/2}$, where q is potential vorticity and θ is potential temperature, the prime indicates zonal mean perturbation, Lait [1994]). The result is typical for January. The FVGCM shows weak tropical MPV fluxes above the tropopause, while the FVDAS shows comparatively larger fluxes reaching into the tropics. The larger MPV fluxes are consistent with the signature of excessive tropical - mid-latitude exchange, and since the FVGCM is the dynamical core of the assimilation system, the excessive fluxes must be originating from the assimilation processes.

The existence of the anomalous tropical PV fluxes suggests excessive EP flux convergence in the tropical region. The flow deceleration associated with the flux convergence would increase the upwelling circulation and increase the overall stratospheric overturning rate. Thus both the weak tropical barrier along with a faster overturning rate would bias the mid-latitude mean age toward the young side.

4.0 Summary and Discussion

From the comparison of DAS and GCM age spectra using trajectory and CTM methods we have concluded:

- 1) Even using the same meteorological data set, the trajectory computed mean ages can differ by a year or more depending on whether the trajectory vertical transport is kinematic or diabatic. This conclusion is similar to the findings of E2000.
- 2) The CTM's and the kinematic trajectory models using DAS fields produce too much vertical dispersion as evidenced by lack of an age spectrum offset at all latitudes and by comparison with the diabatic trajectory calculations. This lack of offset shifts the mean age toward younger values.
- 3) The DAS meteorological fields excessively ventilate the tropics as evidenced by the long tail in the diabatic trajectory age spectra. The ventilation of the tropics allows the mixing of older air into the tropics and younger air into mid-latitudes. Neither observations nor dynamical considerations support the rapid tropical – mid-latitude exchange generated by the DAS meteorological analyses.

- 4) The diabatic and kinematic trajectory age spectra show considerable structure in the DAS calculations. These features can be linked to annual and inter-annual variability in the tropical heating rate. The age spectrum structure becomes more pronounced at middle and high latitudes. The presence of this structure calls into question the stationarity assumption in deriving the Green's function. Interestingly, the CTM produced spectra show almost no structure which we attribute to be a result of transport model diffusion.
- 5) The age offset and tropical ventilation compensate in the kinematic experiments to produce reasonable mean ages in the tropics. This underlines the danger of simply using the mean age as a diagnostic of the circulation. In the mid-latitude and polar regions, the vertical dispersion and tropical exchange work together to produce a very young mean age.
- 6) If the vertical dispersion of particles seen in the kinematic calculations is reduced through the use of diabatic transport, then the tropical mean age is increased by about a year to an unrealistically high value. This is because of the excessive meridional dispersion – the basic lack of a tropical barrier to transport in the DAS, as discussed in Point (3).
- 7) Transport in the FVGCM appears to be more realistic than in the assimilated datasets, even using the kinematic trajectories. The tropical age spectrum shows a reasonable offset and the polar mean age appears to be closer to observations. This result, combined with the results in E2000, suggests that the FVGCM formulation produces more realistic vertical wind fields and improved tropical isolation. Comparing the potential vorticity fields generated by the FVGCM and FVDAS, it appears that the ventilation of the tropics is due to the assimilation process since it is not present in the assimilation core GCM.
- 8) The CTM experiments generally agree with the kinematic trajectory experiments except for the following points: (a) The trajectory experiments show significant structure or anomalies in the age spectrum which is not seen in the CTM spectrum. These anomalies in the spectral tail can be traced to the year-to-year variability in the tropical vertical heating rate. (b) The smoothness of the CTM spectrum suggests additional numerical diffusion is present in the transport scheme that erases the spectrum anomaly structure. It is possible that this extra smoothing creates additional biases in the age spectrum.

Do these results mean that the assimilation analyses are not suitable for stratospheric transport studies? For long-term studies, the answer is probably yes. For short term calculations (weeks – months) the biases are probably not as important although specific tropical – mid-latitude exchange events may show excessive transport.

Another important consideration is the impact of the transport biases we have found on chemical assimilation. Since no observing system will retrieve all the stratospheric constituents, many species will be transported without an observational update. For

example, some of the halocarbon source gases will not be observed by any current or planned satellite system. As the chemical assimilation model runs, these gases will be moved to mid-latitudes and high latitudes too rapidly. Thus the inorganic chlorine, for example, will be underestimated since the source gases will not have time to photolyze.

The failure of the DAS to maintain the tropical barrier to transport in the lower stratosphere appears to be due to the assimilation process. Clearly the GCM is being torqued heavily by the observations and the model is responding with increased wave activity. The dissipation of those waves is probably creating additional, unrealistic tropical ventilation, and may also be accelerating the overall transport circulation through the input of easterly momentum input into the tropics. (The easterly eddy acceleration increases the zonal mean tropical upwelling wave forcing as is seen in the easterly shear phase of the quasi-biennial oscillation.) It is clear from the work of Neu and Plumb [1999] that increasing tropical barrier and a slow down of the overall tropical circulation are both needed to increase the absolute trace mean age in the lower, mid-latitude stratosphere. This line of reasoning suggests that improvements in the model tropical physics will likely reduce the assimilation generated Rossby waves and improve the overall DAS transport characteristics.

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Figure Captions

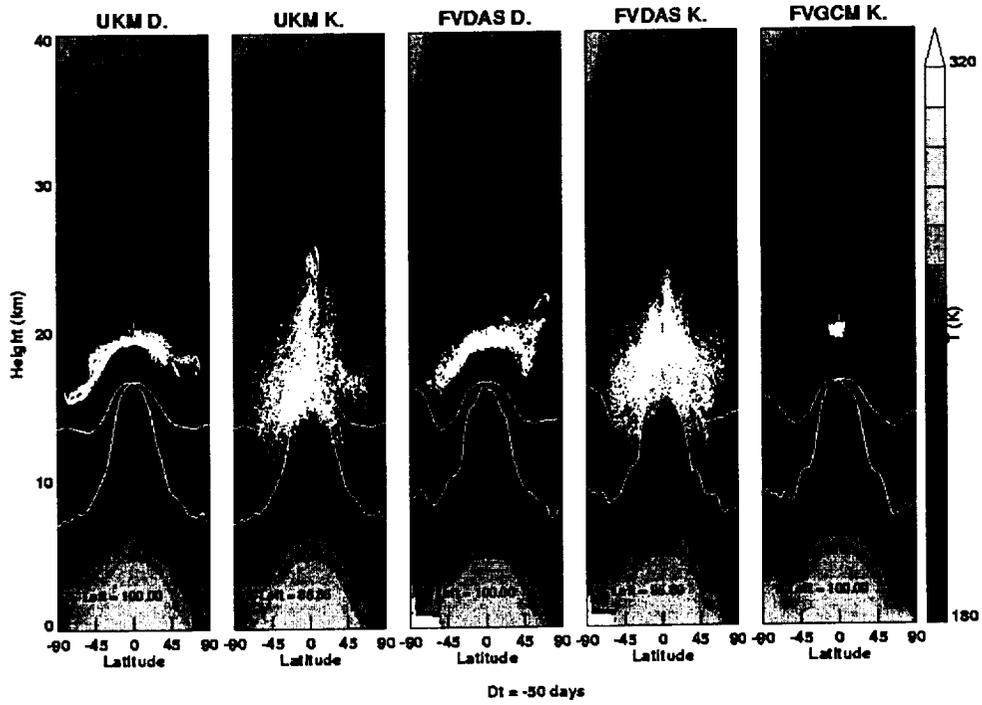


Fig. 1a

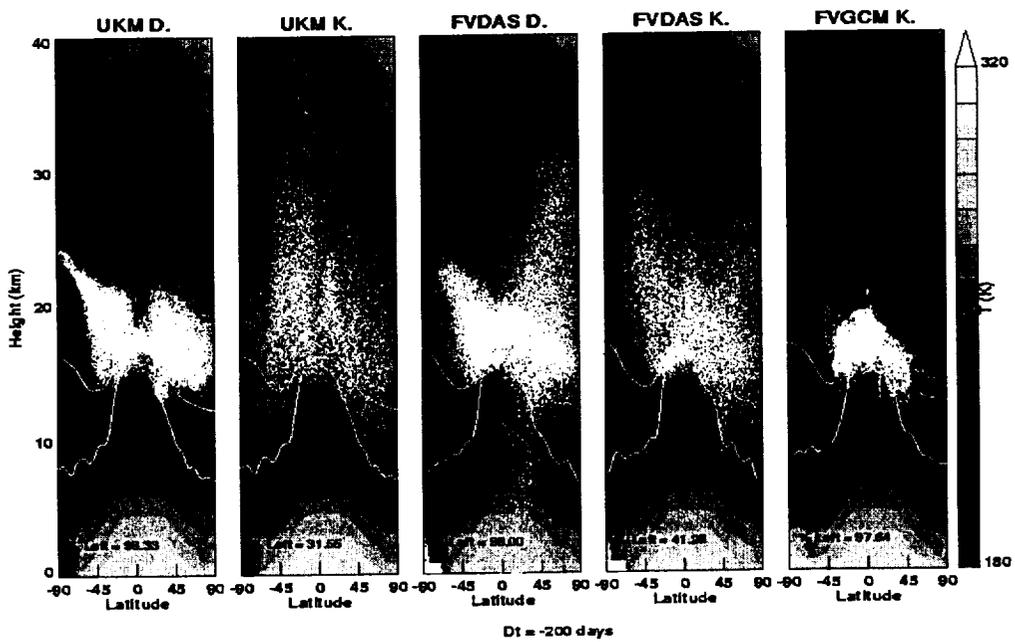


Fig. 1b

Figure 1. The distribution of parcels 50 days (part a) and 200 days (part b) after the beginning of the back trajectory calculation ($Dt = -50, -200$ days). The lower thin white lines show the zonal mean altitude of the tropopause, the upper thin white line shows the zonal mean altitude of the 380K isentrope. The short thin vertical gray line segment at 20 km in each figure over the equator shows the initial position of the parcels. Gray scale indicate zonal mean temperature. Parcels are shown as white dots. The far left panel shows the results using the UKMO DAS wind fields, diabatic trajectories (UKM D). The next panel (left to right) uses the same wind fields, but is a kinematic trajectory calculation (UKM K.). The third panel uses the FVDAS wind fields and diabatic trajectories (FVDAS D.). The fourth panel uses the FVDAS with kinematic trajectory calculation (FVDAS K.). The fifth panel shows the kinematic trajectory calculation using the FVGCM (FVGCM K.). The percent of parcels remaining in the stratosphere at the time are indicated in each panel.

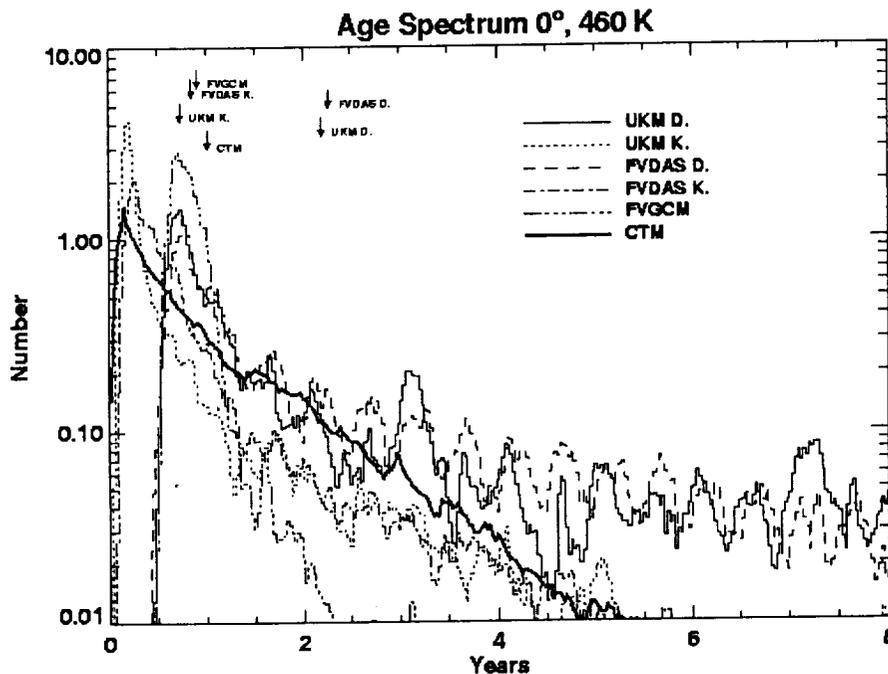


Figure 2 The normalized age spectrum for the tropical experiments (Table 1). UKM D. indicates diabatic trajectories using the UKMO DAS. UKM K is the kinematic trajectory calculation. FVDAS D is the diabatic trajectory calculation using the FVDAS data set, and FVDAS K is the kinematic calculation. FVGCM is the GCM calculation using kinematic trajectories. Small arrows locate the mean ages. The thick line indicates the CTM age spectrum using UKMO DAS.

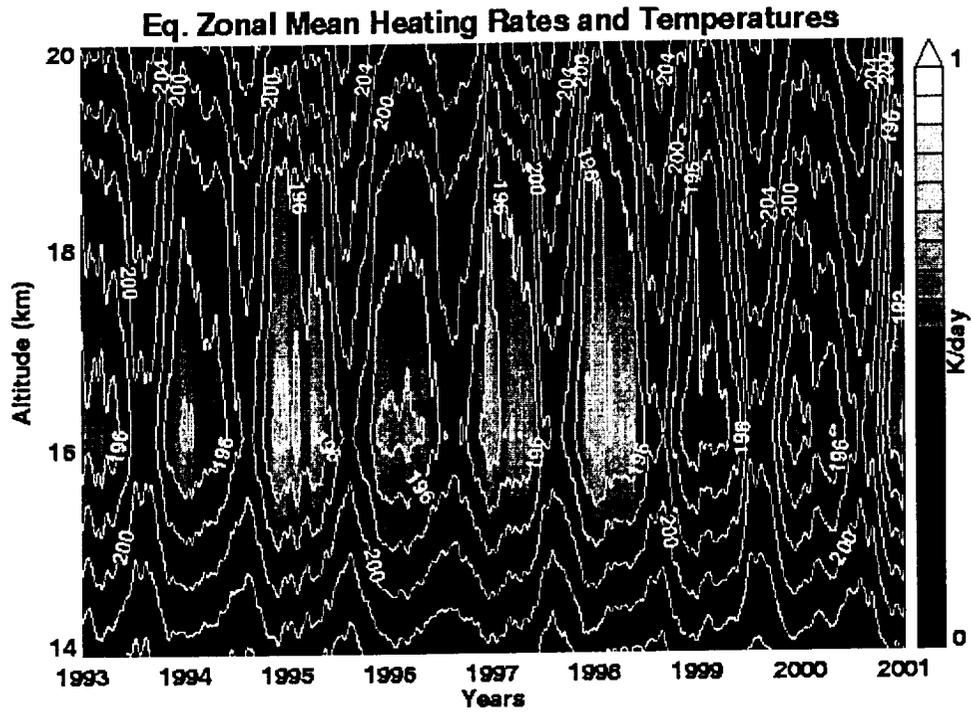


Figure 3 Time series of the tropical heating rates computed for the UKMO DAS in deg/day. Contours show the tropical temperatures in degrees K.

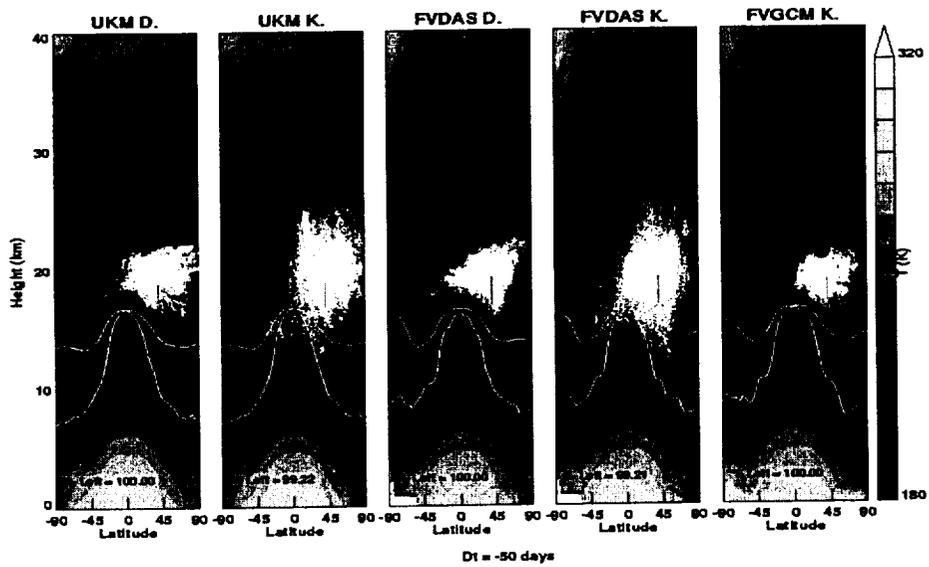


Figure 4a

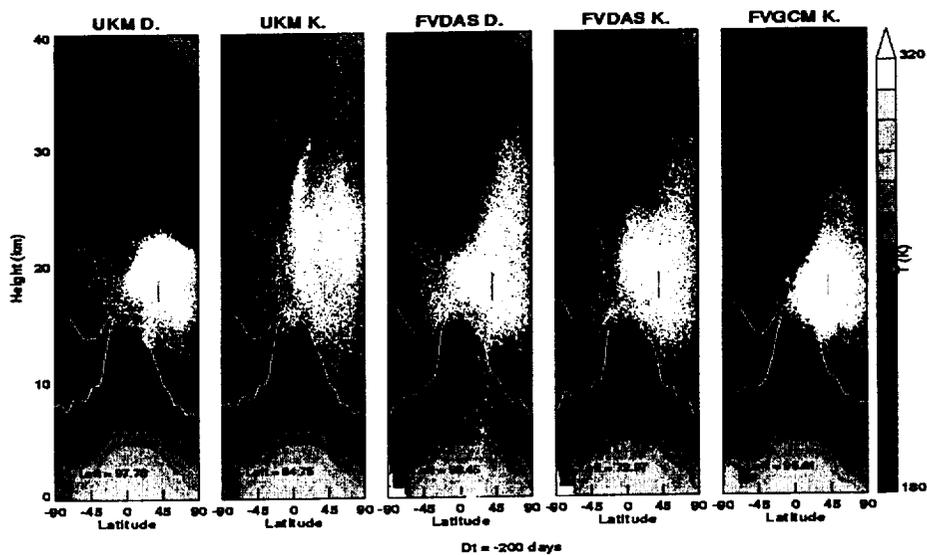


Figure 4b

Figure 4. Same as Figure 1 except for 40° N release.

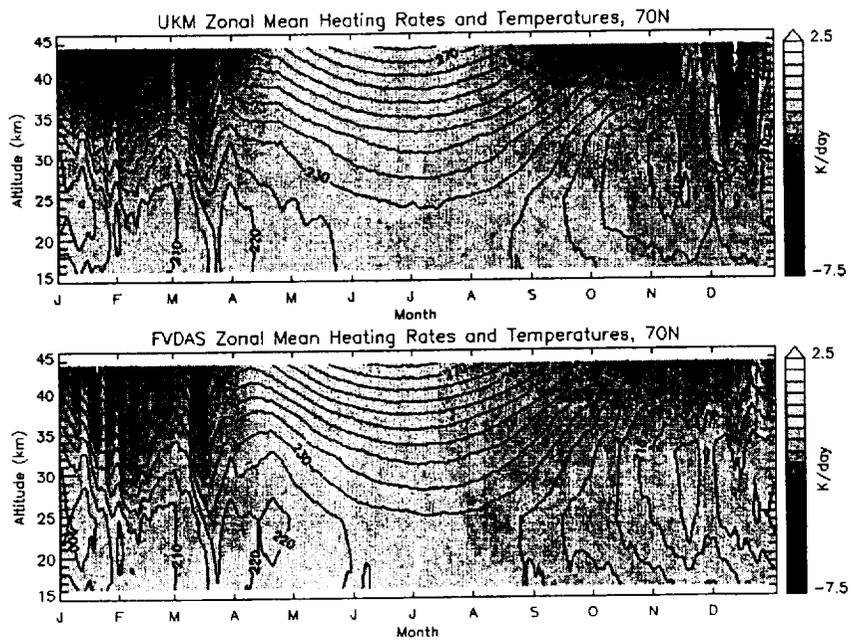


Figure 5 Comparison of the zonal mean net heating rates and temperatures at 70° N from the UKMO and FVDAS assimilations. Temperature contours in black, heating rates are color coded as indicated on the right color bar. The white contour indicates zero heating.

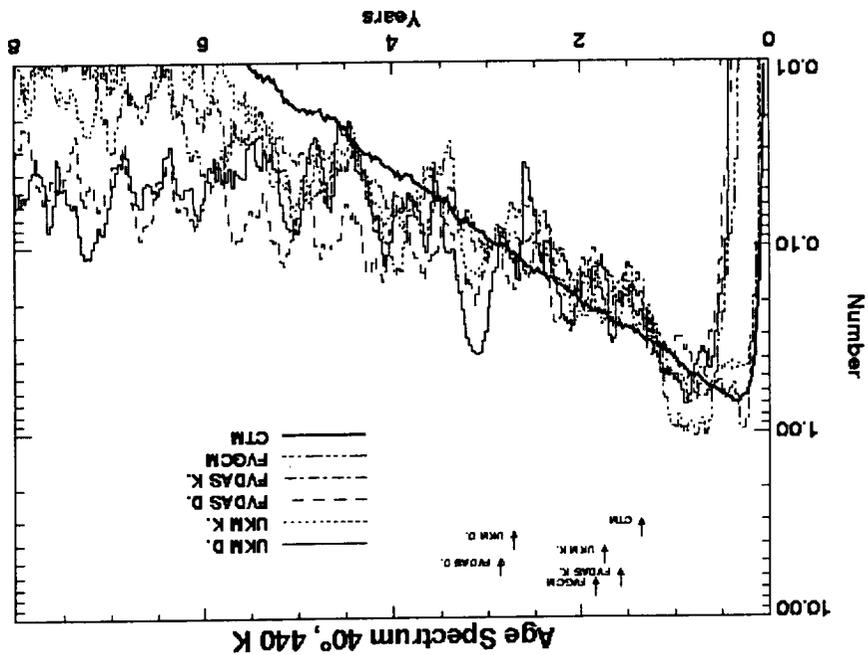


Figure 6 Same as Figure 2 for 40° release.

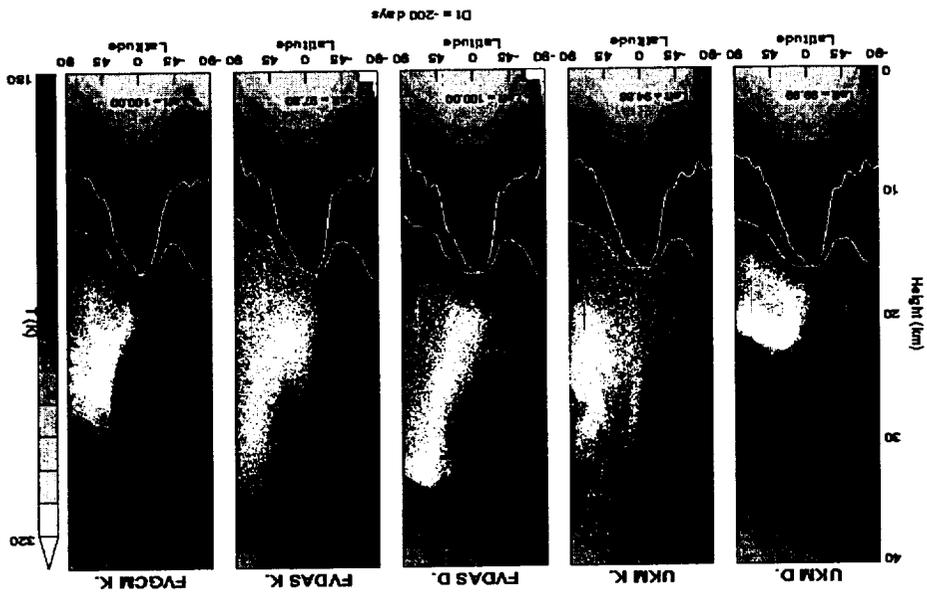


Figure 7 As in Figure 1b except for a release at 70° N.

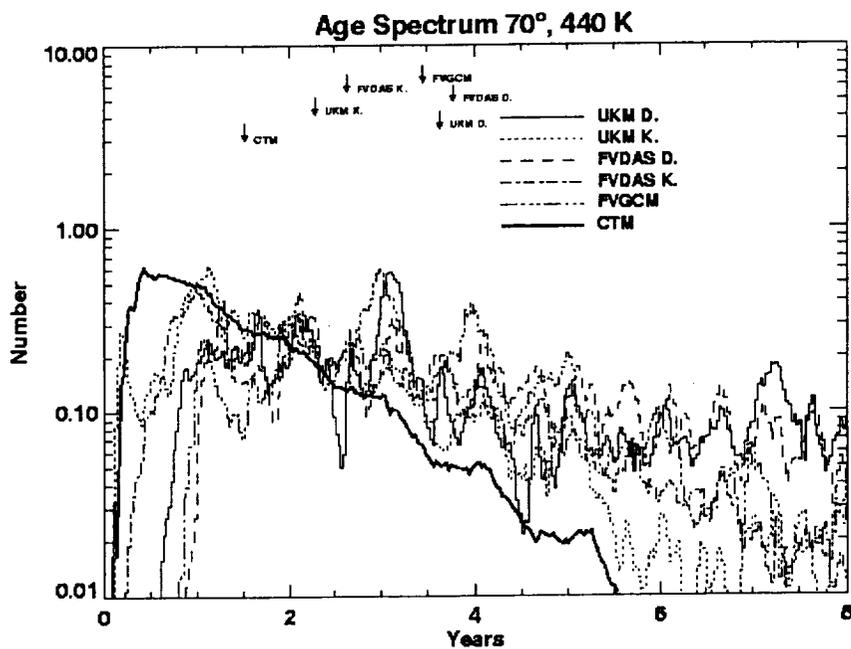


Figure 8 The age spectrum for the 70° N release experiment. See Figure 2 for details.

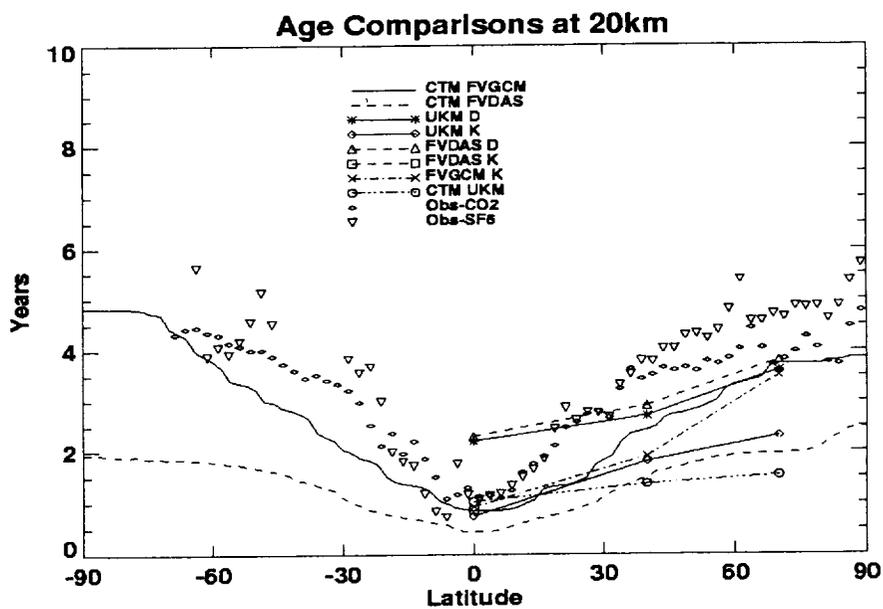


Figure 9. Summary of mean ages from models and observations. Dashed line is mean age estimated from the CTM using FVDAS winds. Solid line is mean age estimated from the CTM using FVGCM winds. Both mean ages are derived from an SF₆ type increasing tracer experiment. Trajectory and CTM pulse experiment age estimates are indicated in the legend and are shown as symbols connected with lines. Mean ages from ER-2 observations of CO₂ and SF₆ are indicated by symbols from Hall et al. [1999]. All mean ages are taken from the tropopause.

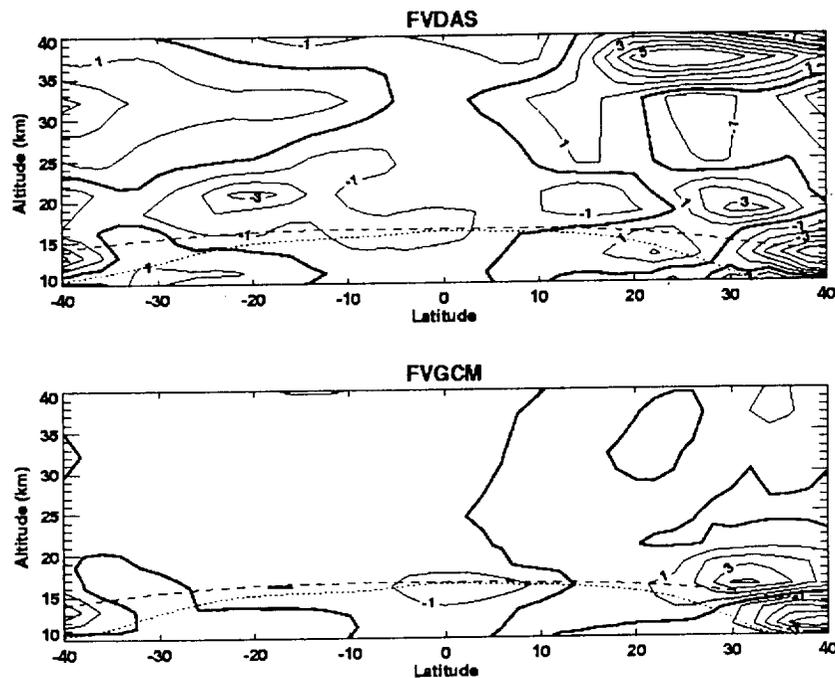


Figure 10. Comparison of the tropical zonal mean MPV flux for January 2000 in the FVDAS (upper panel) and January for a year in the FVGCM (lower panel). Units are $10^6 \text{ K m}^3/\text{kg/s}^2$. The dashed line shows the zonal mean 380K potential temperature surface. The dotted line is the zonal mean tropopause.